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BENCHTOP INSENSITIVITY: FIRST STEPS WITH PETN (BRIEFING CHARTS)

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CONFERENCE BRIEFING CHARTS

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Benchtop Insensitivity: First Steps with Shocked PETN

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Insensitive Munitions

- "Insensitive Munitions (IM) are conventional weapons and ordnance that fulfill their performance objectives while <u>minimizing collateral damage if exposed to stimuli including fires, impact and shock threats</u>." (emphasis added)

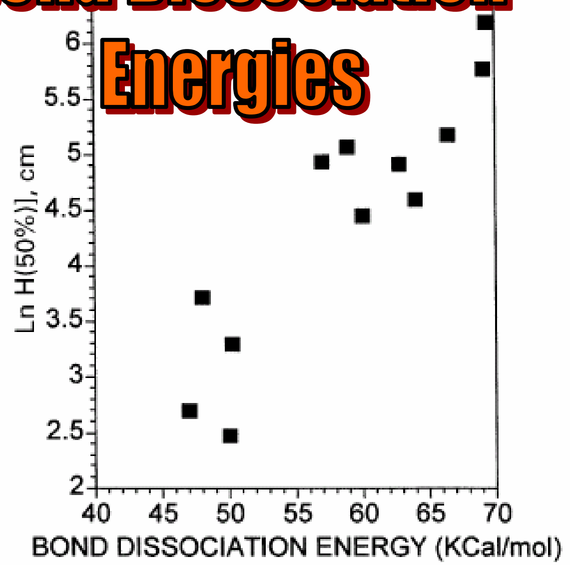
- "The statutory requirement for IM is set forth in U.S. Code, Title 10, Subtitle A, Part IV, Chapter 141, Section 2389..."

Department of Defense Acquisition Manager's Handbook for Insensitive Munitions
January 2004, Revision 01

Many Influences on Sensitivity

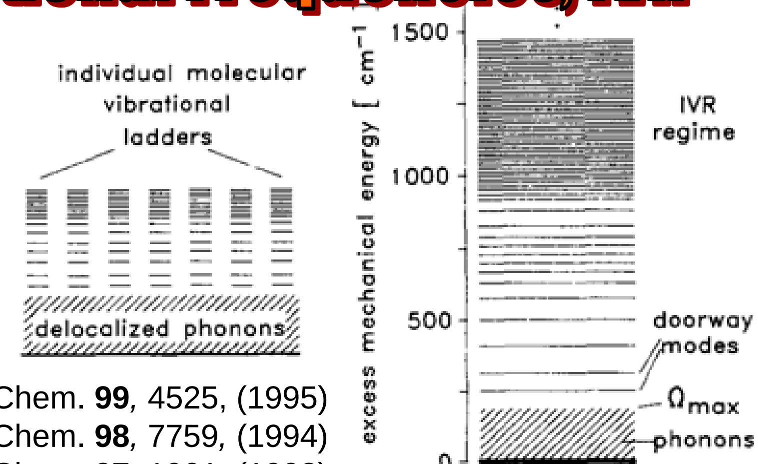
Voids and defects

Bond Dissociation Energies



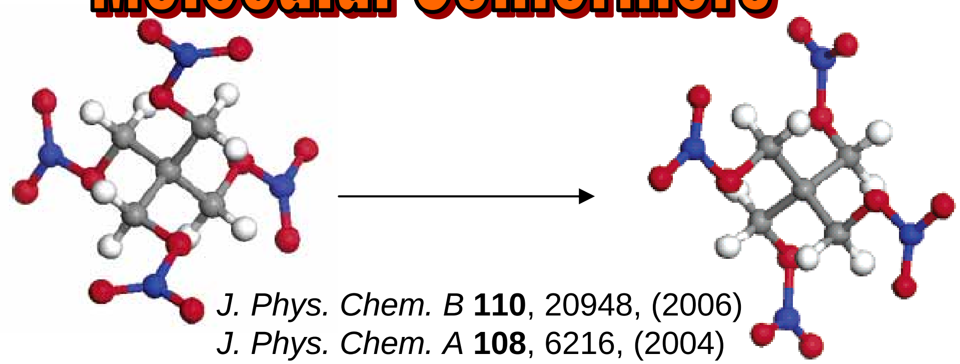
B. M. Rice *et al*, J. Mol. Struc. **583**, 69 (2002).

Vibrational Frequencies, IVR



J. Phys. Chem. **99**, 4525, (1995)
J. Phys. Chem. **98**, 7759, (1994)
J. Phys. Chem. **97**, 1901, (1993)
J. Chem. Phys. **92**, 3798, (1990)

Molecular Conformers

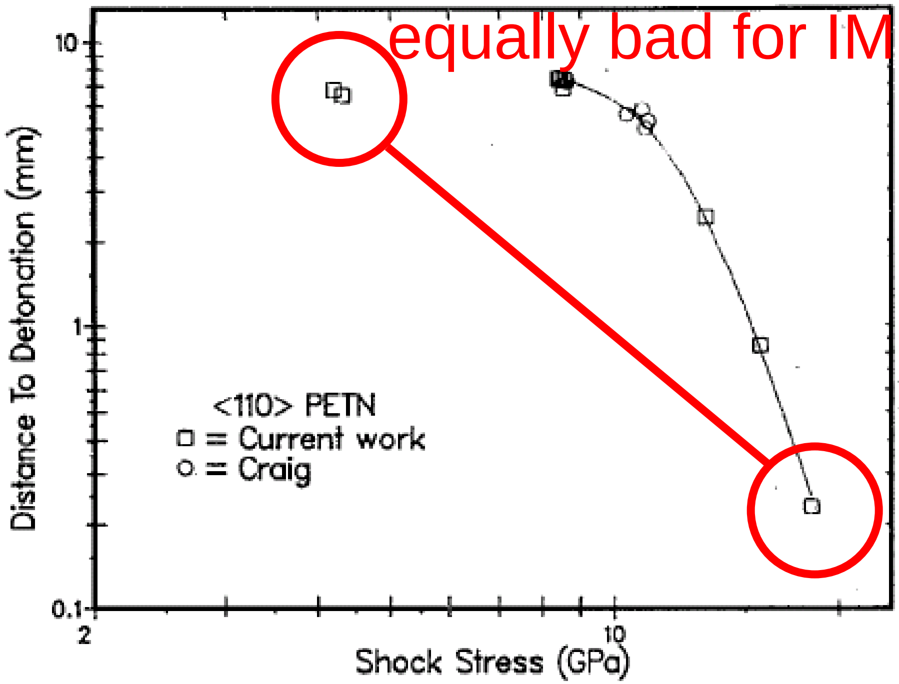


J. Phys. Chem. B **110**, 20948, (2006)
J. Phys. Chem. A **108**, 6216, (2004)

"Initiation" Diagnostics

- Flash of light
- Loud sound
- Dent/hole in a witness plate

} focus on detonation



J. J. Dick *et al*, J. Appl. Phys. **70**, 3572 (1991).

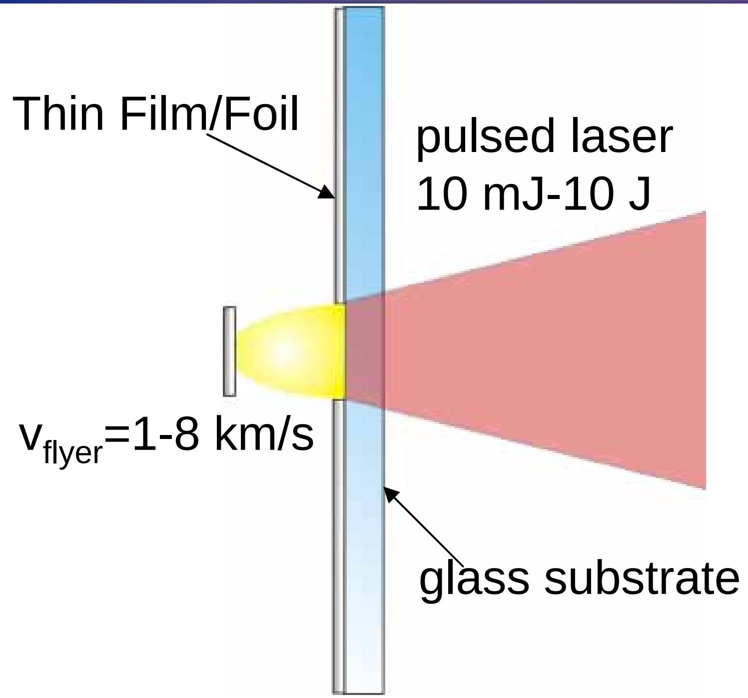
Detonation is scale dependent! Stimuli which will not induce a prompt detonation in a small sample can lead to detonation in a larger one.

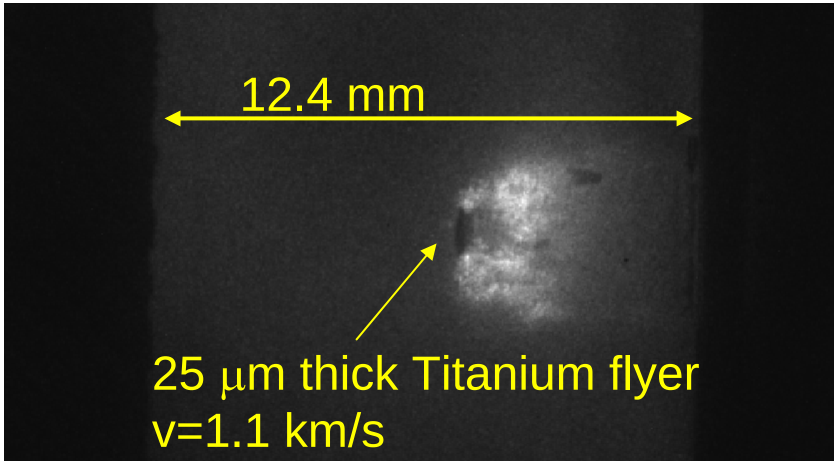
Ideal Diagnostic Wishlist

- Non-Subjective
- Detect initiation of chemical reactions without relying on detonation
- Use small samples

  (Allows rapid exploration of an enormous parameter space influencing sensitivity)
- Reproducible
- Observe reaction intermediates to gain insight into microscopic initiation conditions

Laser-Driven Flyers

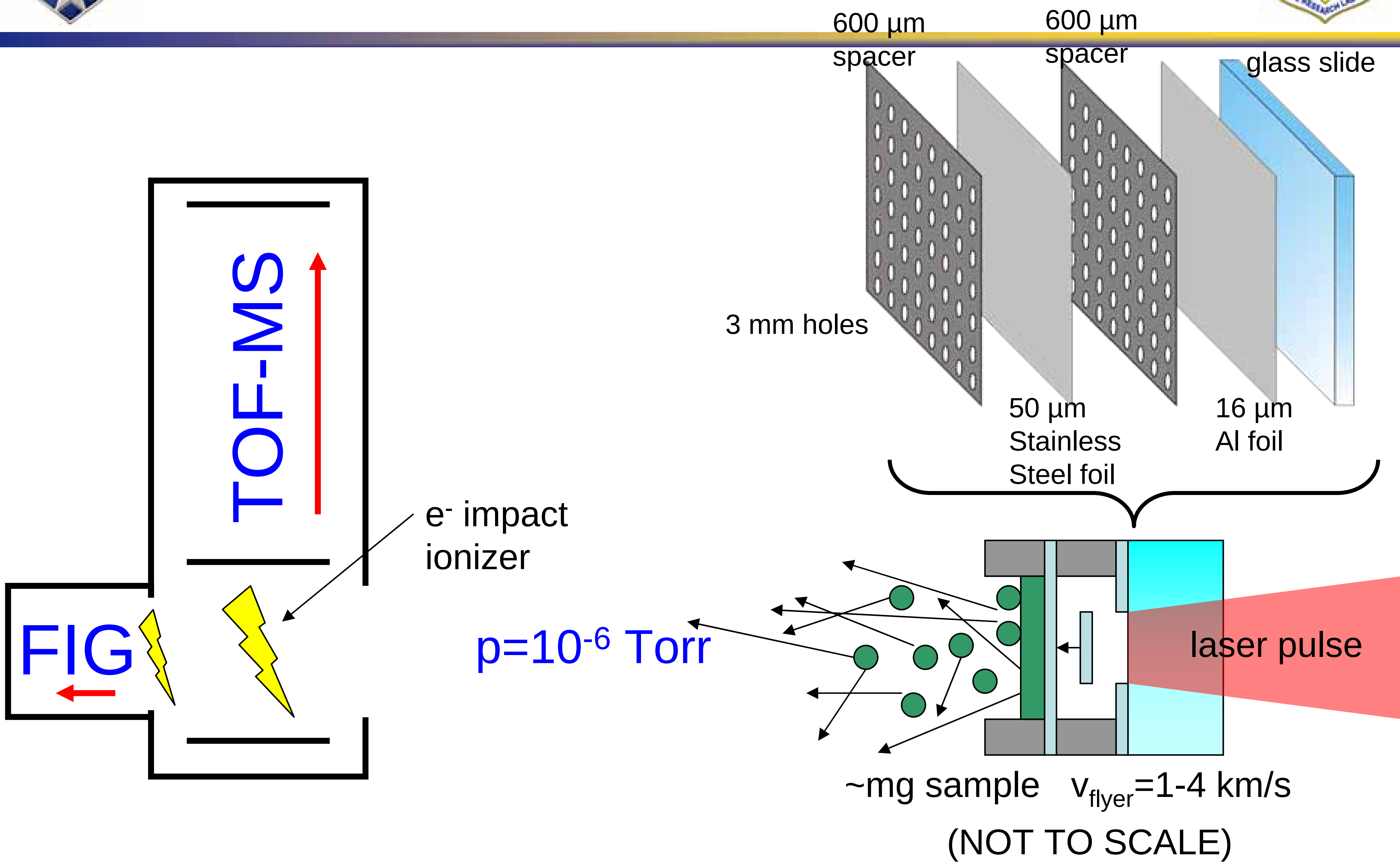




$E_{flyer}/E_{laser} = 0.1\text{-}0.3$

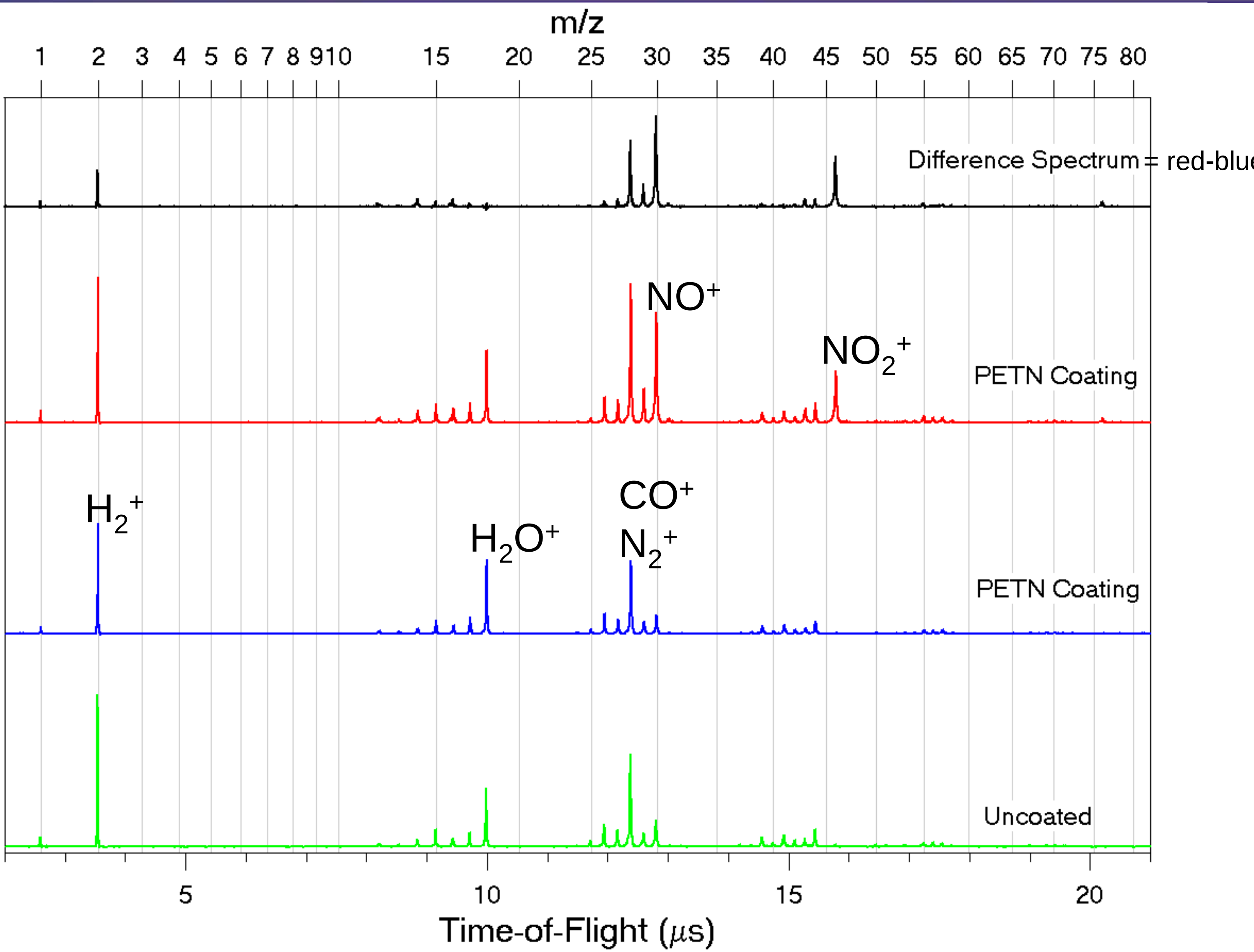
Laser-driven flyers can be used to create rapid, repetitive shocks (0-100 GPa typical).

Experiment

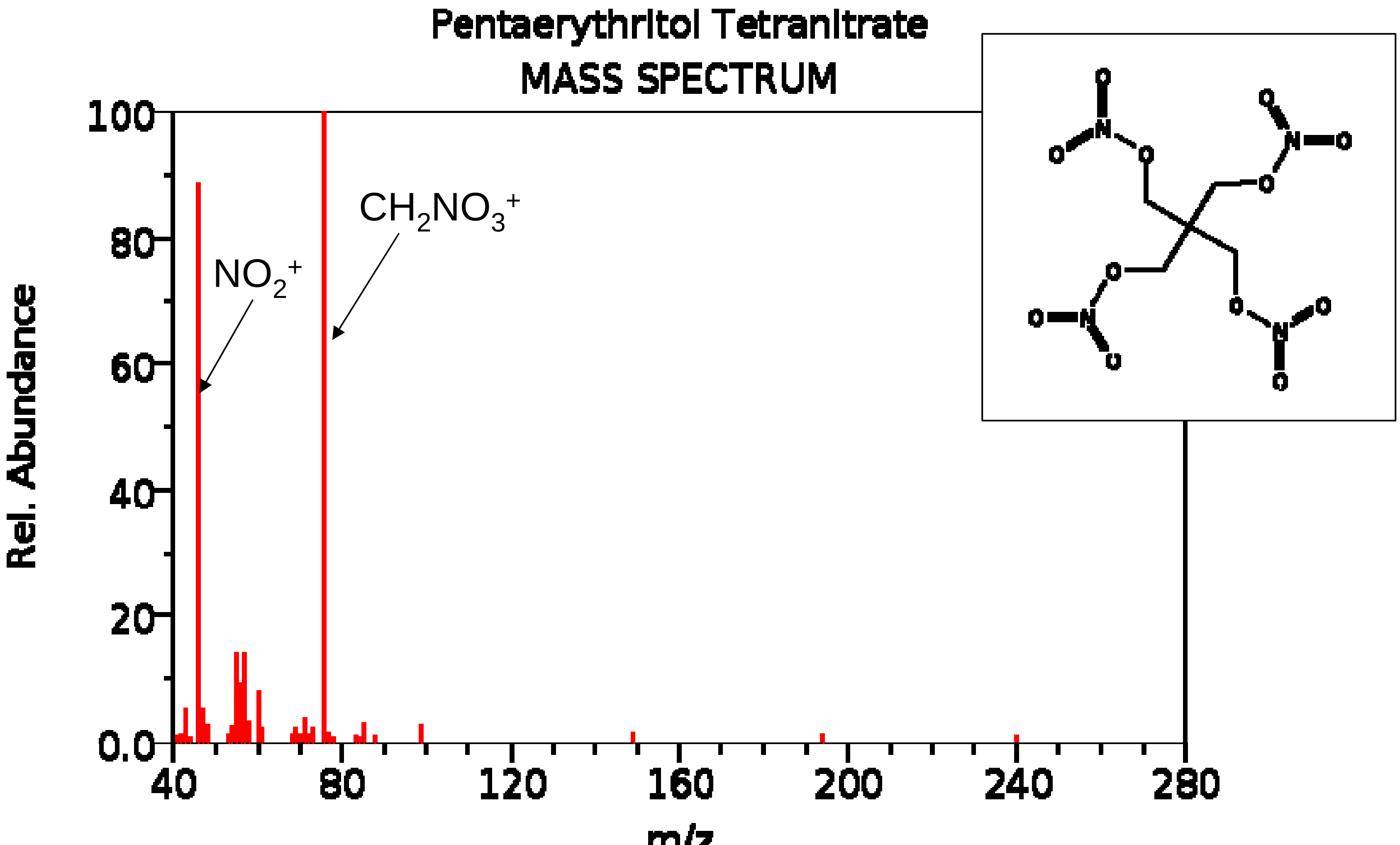


600 µm spacer
600 µm spacer
glass slide
3 mm holes
50 µm Stainless Steel foil
16 µm Al foil
TOF-MS
FIG
e⁻ impact ionizer
p=10⁻⁶ Torr
laser pulse
~mg sample
v_flyer=1-4 km/s
(NOT TO SCALE)

TOF-MS Diagnostic

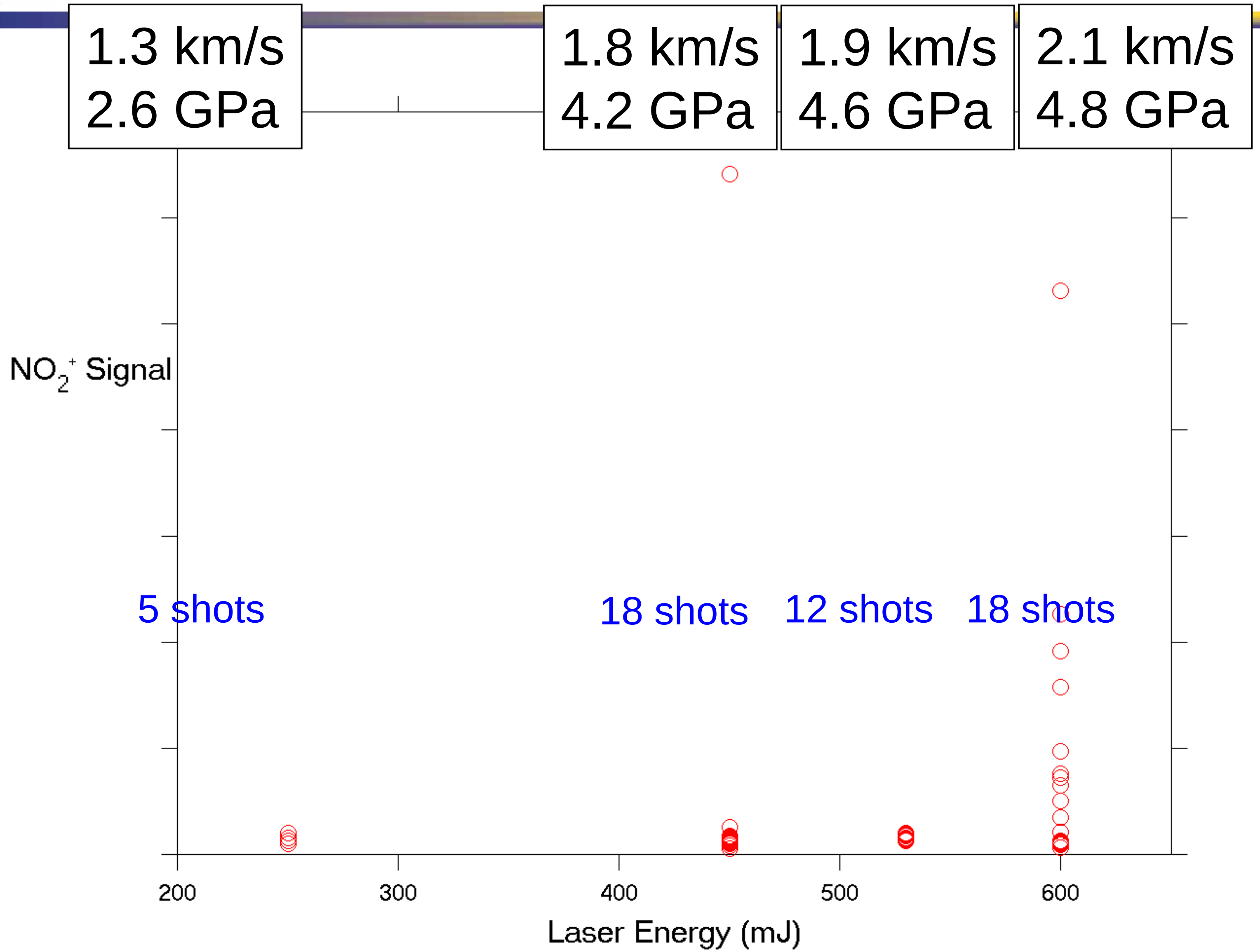


Gas-Phase PETN (Unreacted)



NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

Initiation Threshold (Almost)



Flyer-Induced Detonation

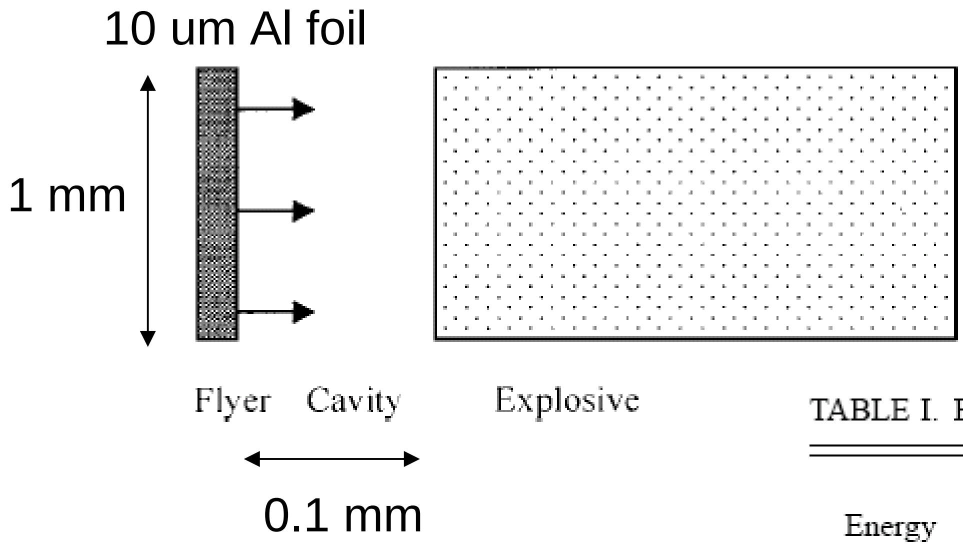


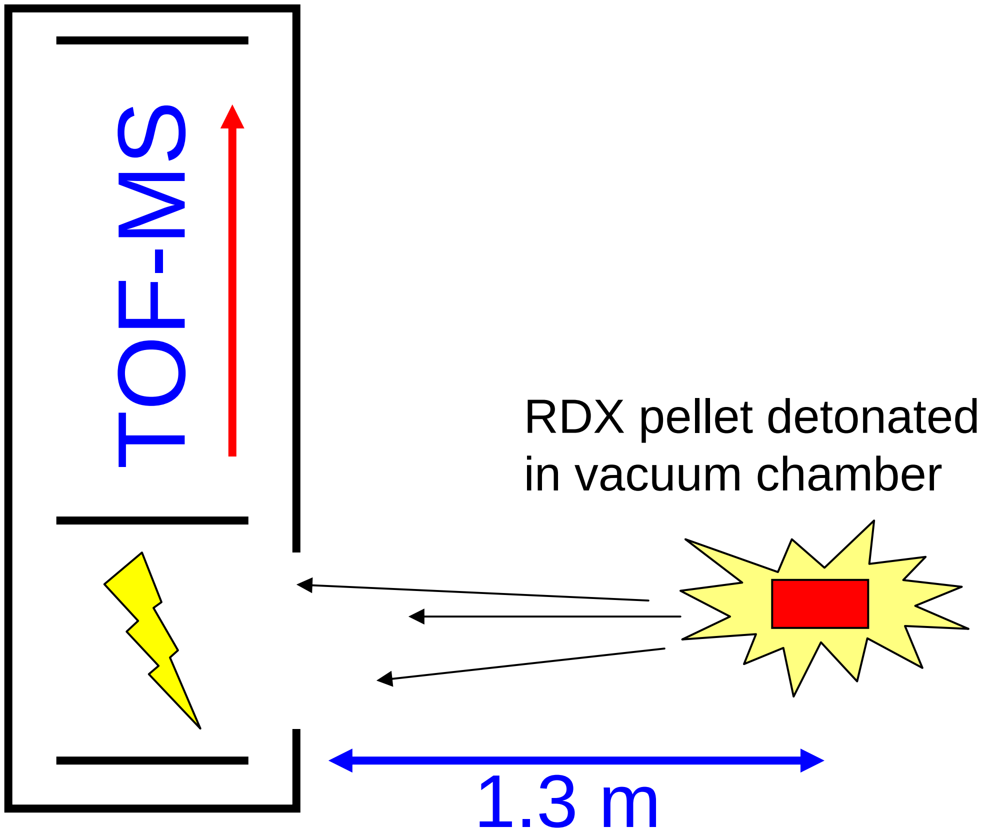
TABLE I. Experimental results of initiating explosive by laser driven flyer.

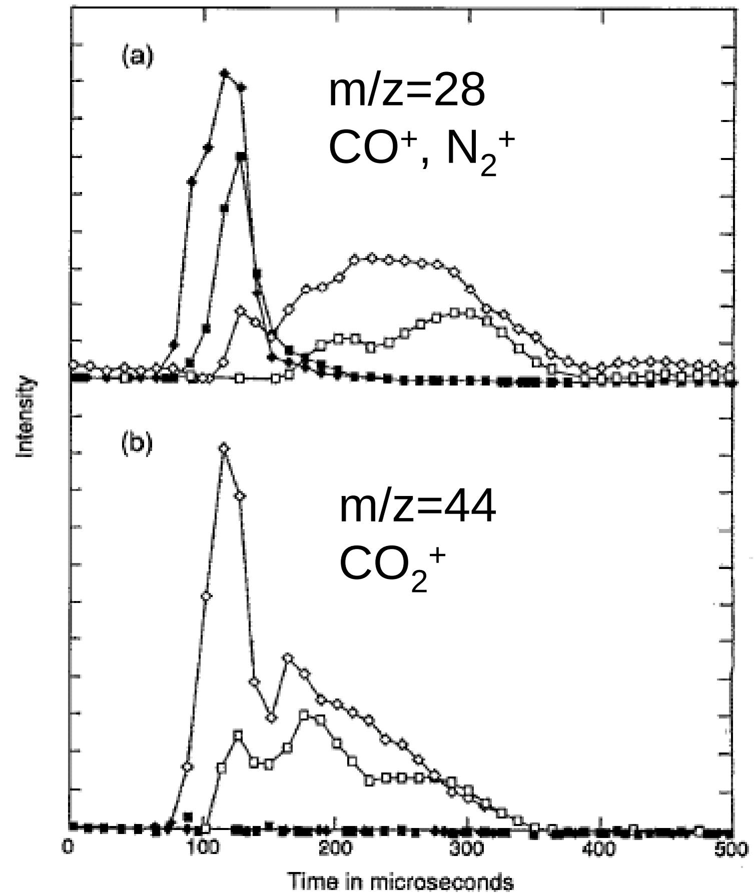
Energy density (J/cm^2)	Velocity of flyer (km/s)	Pulse width (ns)	Impacting pressure (GPa)	Detonation or not
51	3.6	2.1	19.4	Yes
50.6	2.1	3.8	8.1	Yes
48.6	2.0	3.8	7.5	Yes
47	2.0	3.8	7.3	Yes
45	1.9	3.8	6.9	No
44	1.9	3.8	6.8	No
38	1.7	3.8	5.8	No
78	2.8	3.8	12.7	Yes
93	3.1	3.8	15	Yes

Threshold for prompt detonation is ~ 7 GPa

G. Zhouwei, et al, J. Appl. Phys. **96**, 344 (2004).

TOF-MS Detonation Studies

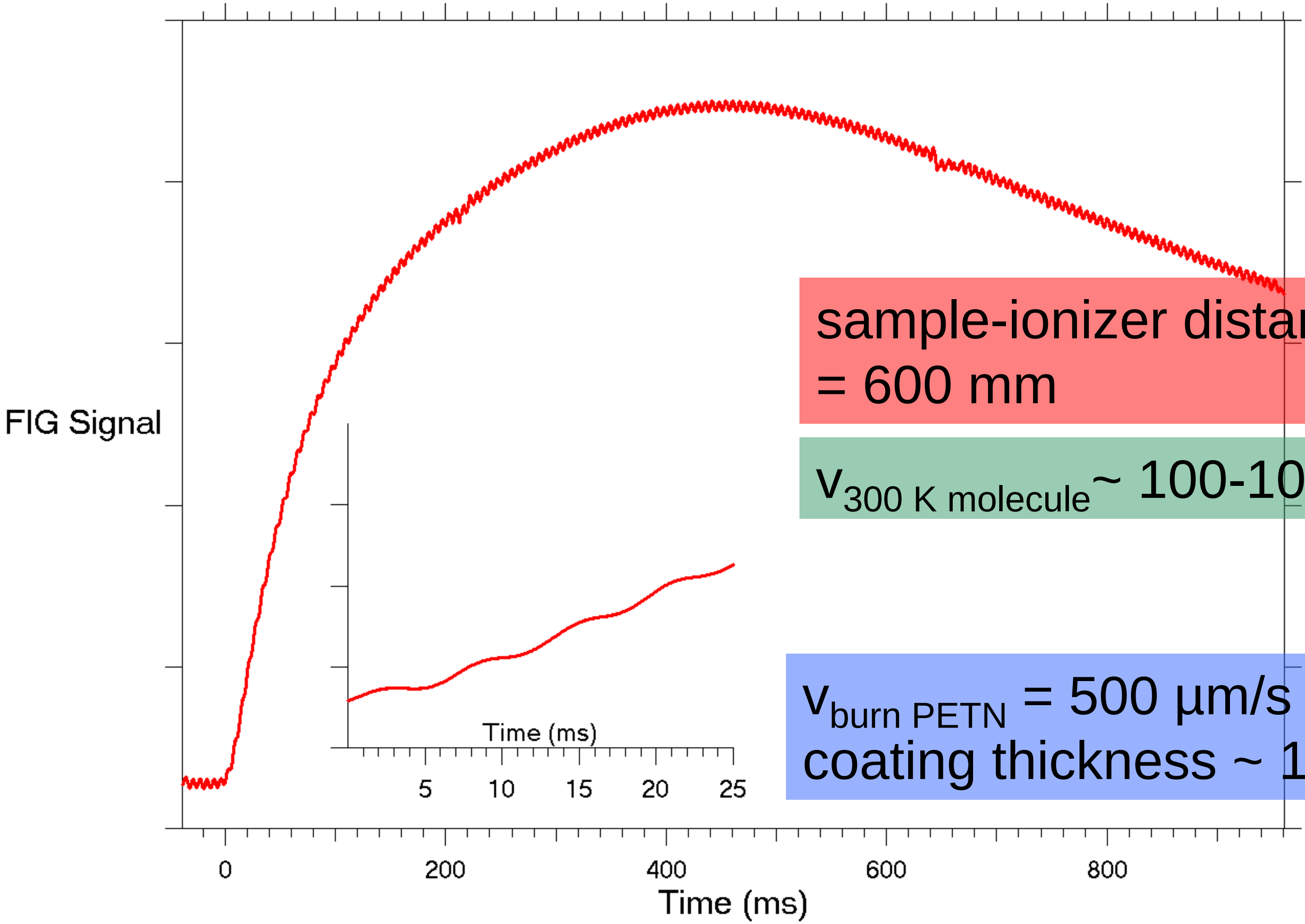




v=4-13 km/s

N. C. Blais, H. A. Fry, and N. R. Greiner, Rev. Sci. Instrum. **64**, 174 (1993).

Time Dependence

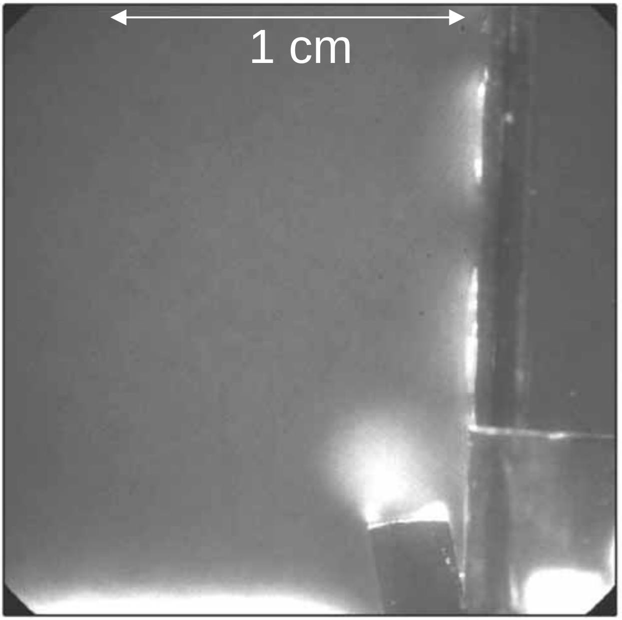


sample-ionizer distance = 600 mm

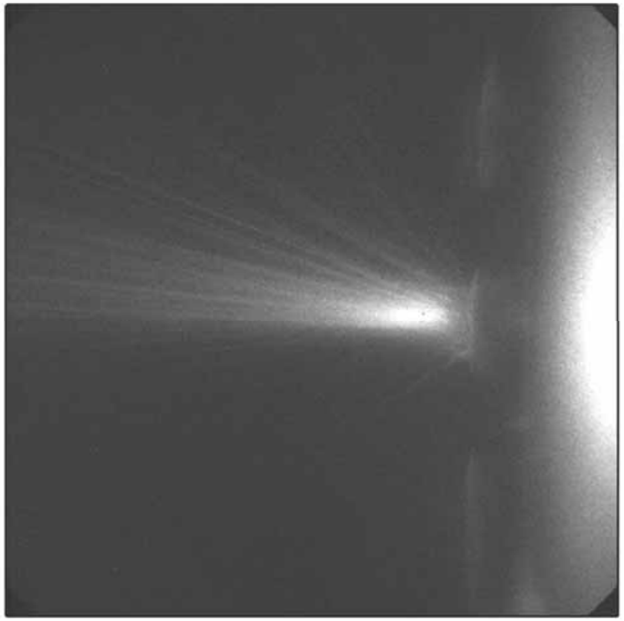
$v_{300\ K\ molecule}$ ~ 100-1000 m/s

$v_{burn\ PETN}$ = 500 μm/s
coating thickness ~ 100 μm

Post-Impact Luminescence



Sample under ambient lighting

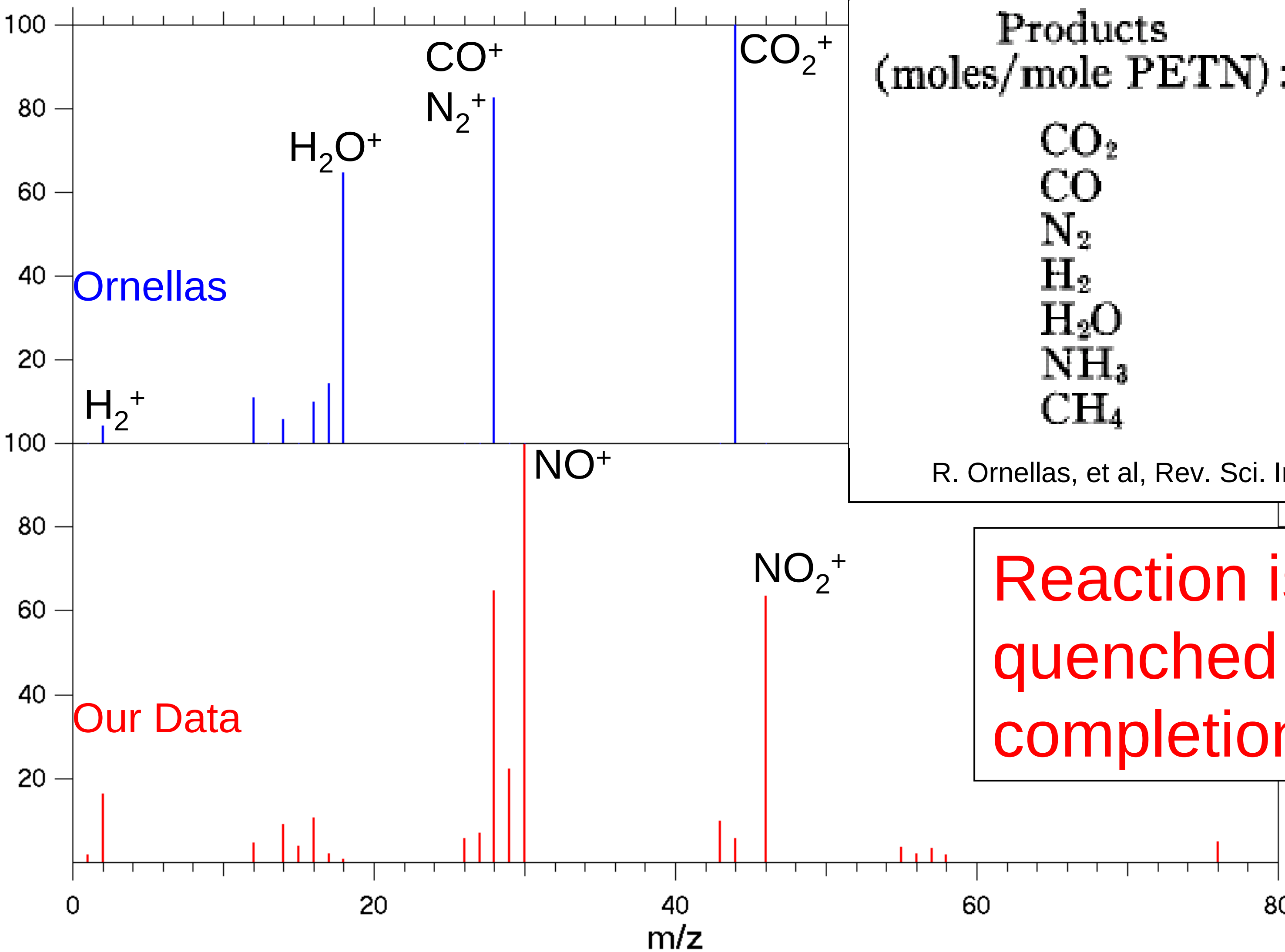


25 ms exposure
50 µs delay from flyer impact

1 ms exposure
7 ms delay from flyer impact

m/s velocities!

PETN Reaction Products



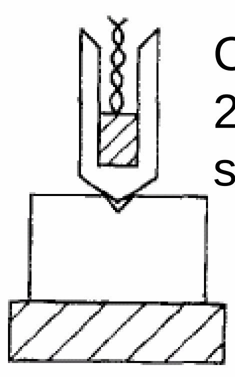
Products (moles/mole PETN):

CO_2	3.50±0.04
CO	1.56±0.08
N_2	2.00±0.04
H_2	0.51±0.04
H_2O	3.45±0.04
NH_3	<0.0002
CH_4	<0.0002

R. Ornellas, et al, Rev. Sci. Instrum. **37**, 907 (1966).

Reaction is quenched before completion

PETN Crystal Fracture



Chisel rapidly driven into 20 mm X 5 mm X 3 mm single crystal

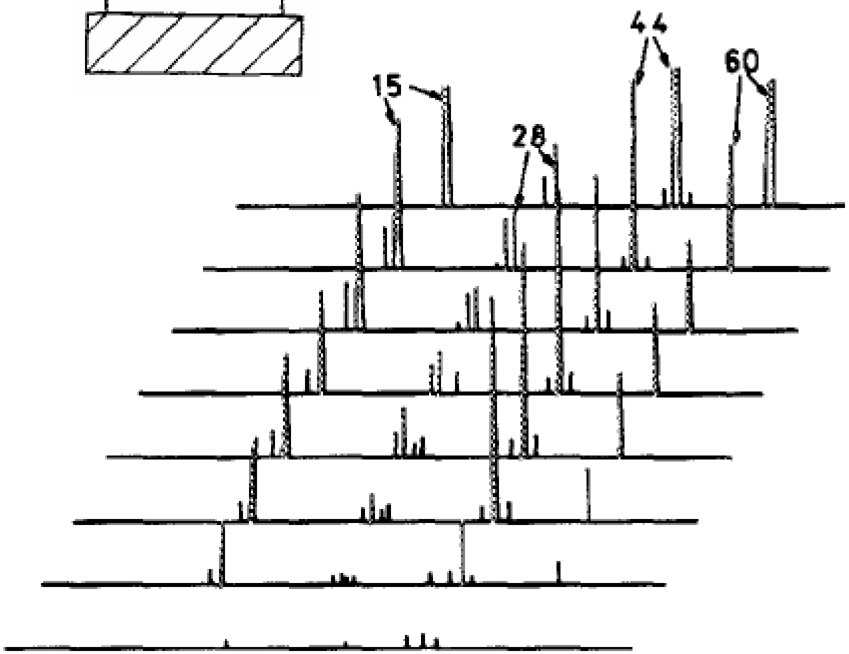
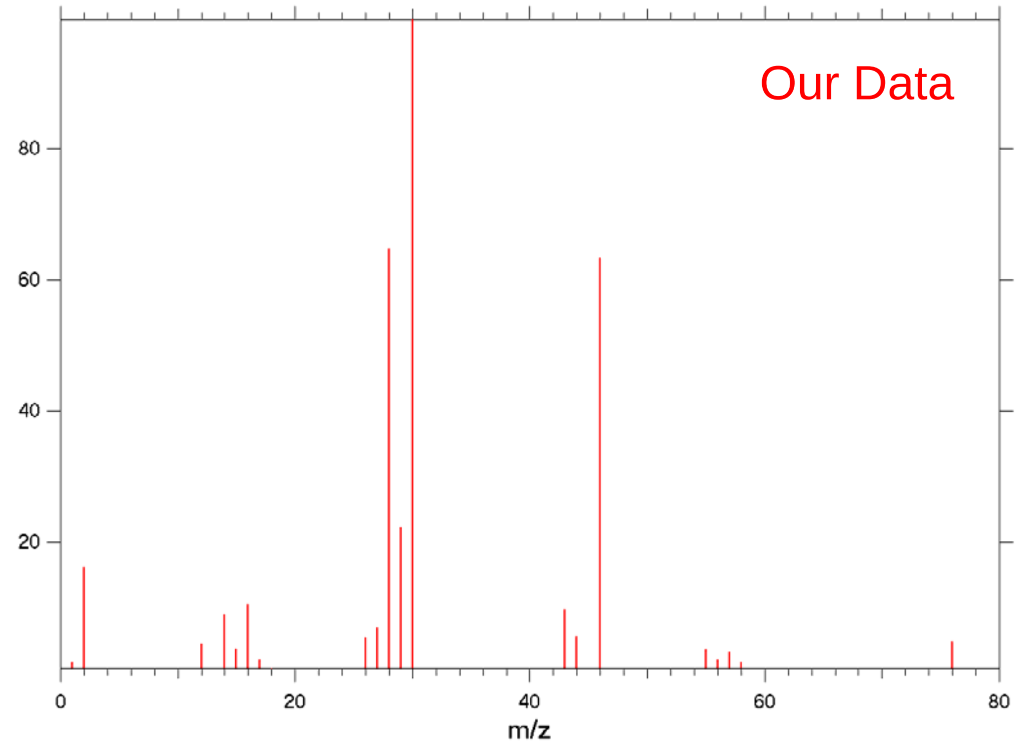


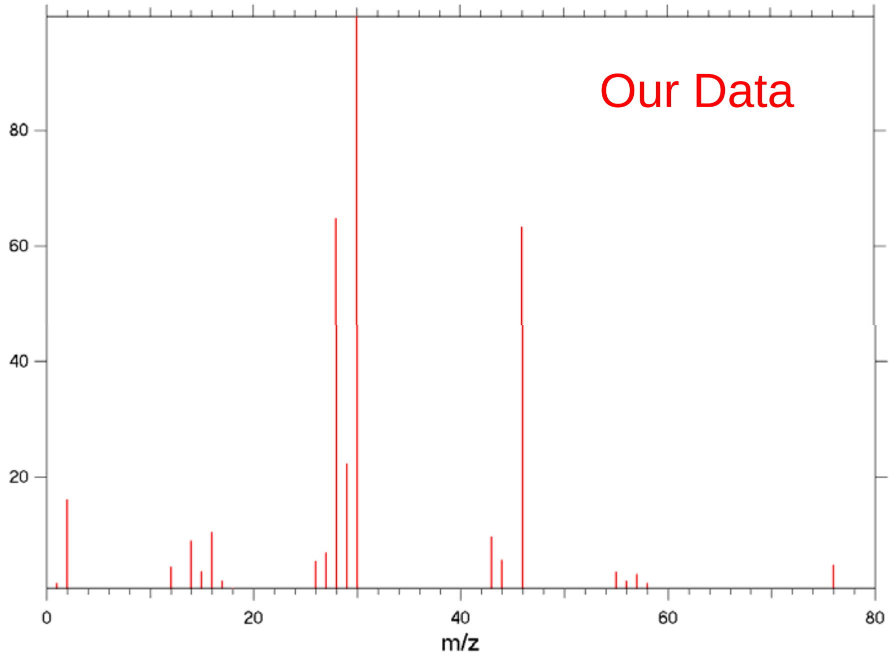
FIG. 5. Complete spectrum for energetic fracture. Time delay 350 μs, 250 μs per step.

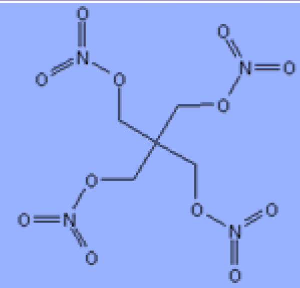
W. L. Ng, J. E. Field, H. M. Hauser, J. Appl. Phys. **59**, 3945 (1986).



Inconsistent with crystal fracture alone

PETN Thermal Decomposition





Prominent peaks at: 18, 28, 29, 30, 44, 46

W. L. Ng, J. E. Field, H. M. Hauser, J. Appl. Phys. **59**, 3945 (1986).

1) $C(CH_2NO_3)_4 \rightarrow C(CH_2NO_3)_3CH_2O + NO_2$

2) $C(CH_2NO_3)_3CH_2O \rightarrow C(CH_2NO_3)_3 + CH_2O$

3) $C(CH_2NO_3)_3 \rightarrow 2\ CH_3NO_3 + 2\ CO + NO$

4) $CH_3NO_3 \rightarrow CH_3O + NO_2$

5) $CH_3O + NO_2 \rightarrow CH_2O + HNO_2$

6) $2\ HNO_2 \rightarrow H_2O + NO + NO_2$

7) $CH_3O + CH_2O \rightarrow CH_3OH + HCO$

8) $HCO + NO \rightarrow CO + HNO$

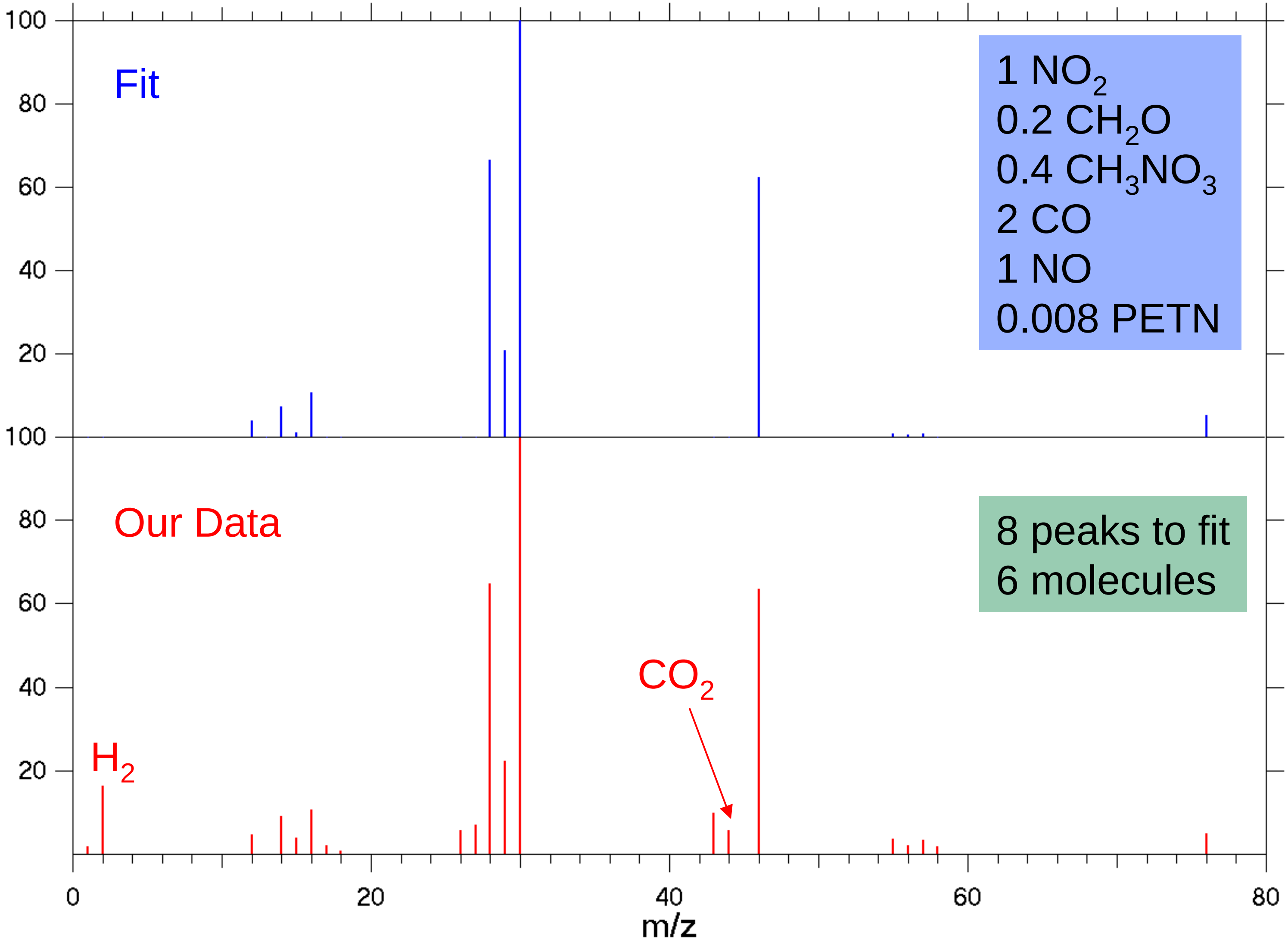
9) $2\ HNO \rightarrow H_2O + N_2O$

Species consistent with our spectrum:
NO_2, CH_2O, CO, NO, N_2O

Species inconsistent with our spectrum:
H_2O, CH_3OH

Mass spectra unavailable:
CH_3O, HNO_2, HCO, HNO

Compare with Thermal Mechanism



Summary

- Developed a technique that can objectively detect chemical reactions in small energetic samples
- Measured an initiation threshold (almost) for PETN samples
- Technique can distinguish initiation from detonation
- Reaction is quenched before it reaches completion
- Observed reaction intermediates are consistent with thermal processes

Future Directions

- Better map-out PETN initiation conditions and reaction kinetics
- Extend measurements to other explosive substances
- Compare measured sensitivities with results from more traditional diagnostics
- Incorporate spectroscopic techniques to measure energy content of observed species